Supporting Information

Two Polymorphs and Cocrystal of Styryl-pyridine Derivatives with Tuned Emission Induced by Co^{2+} and $Zn(phen)_3^{2+}$

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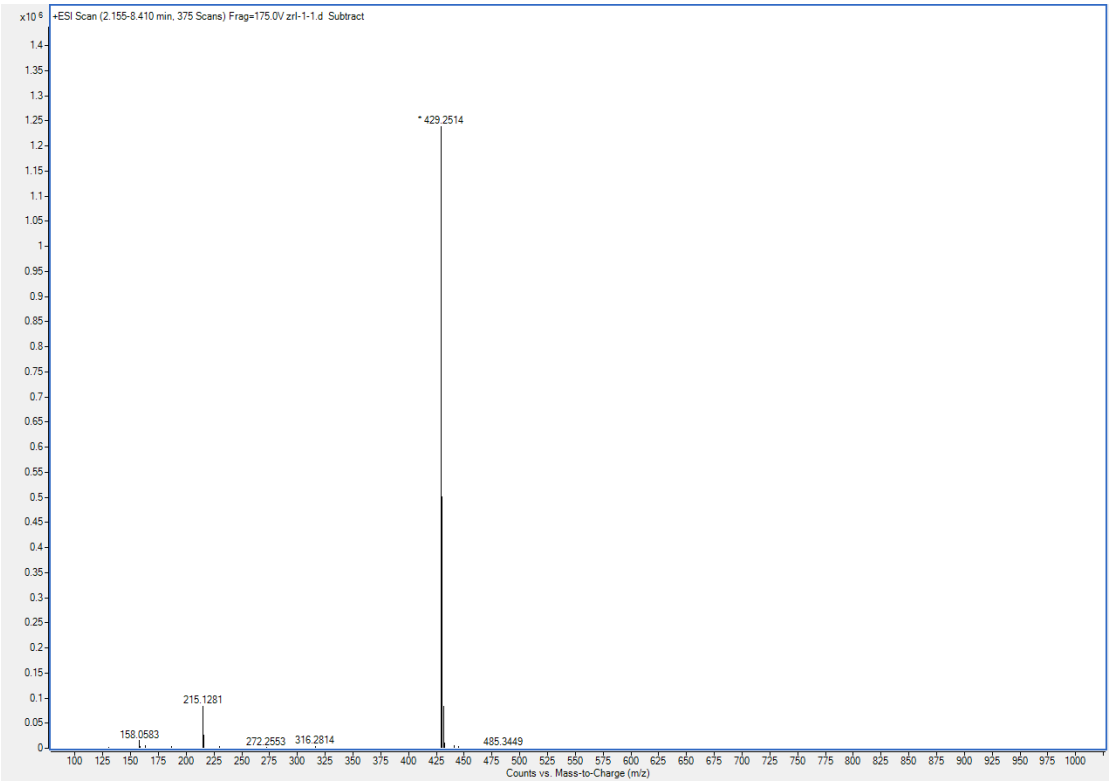


Fig. S1 HRMS spectrum of compound **L**

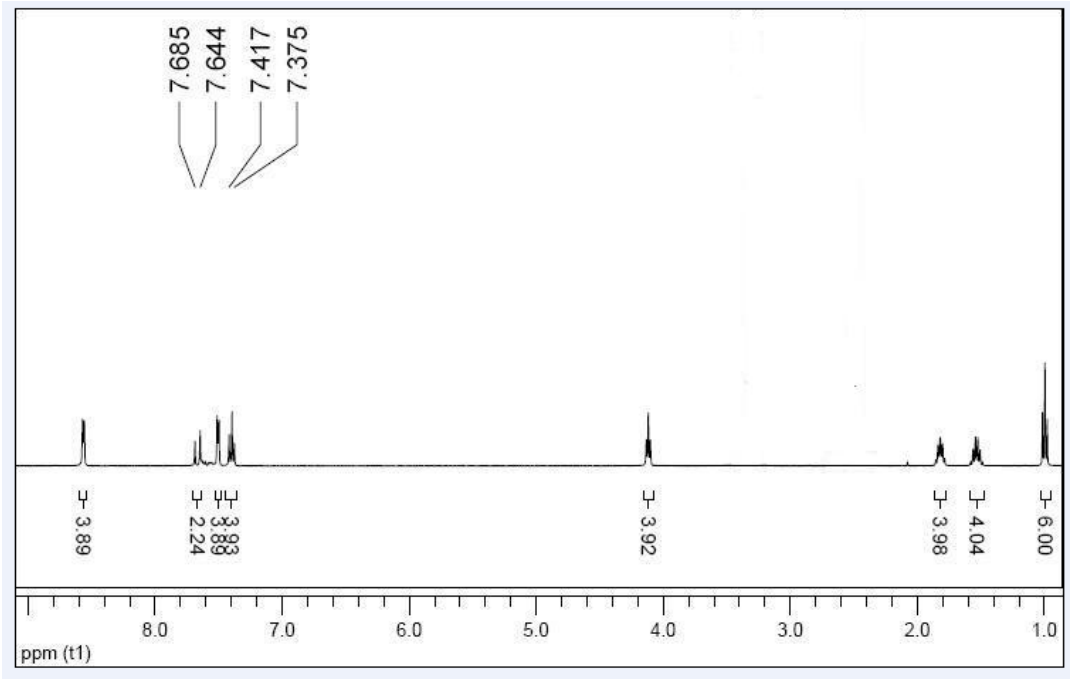


Fig. S2 ^{1}H NMR (d_6-DMSO, 400 MHz) of compound L

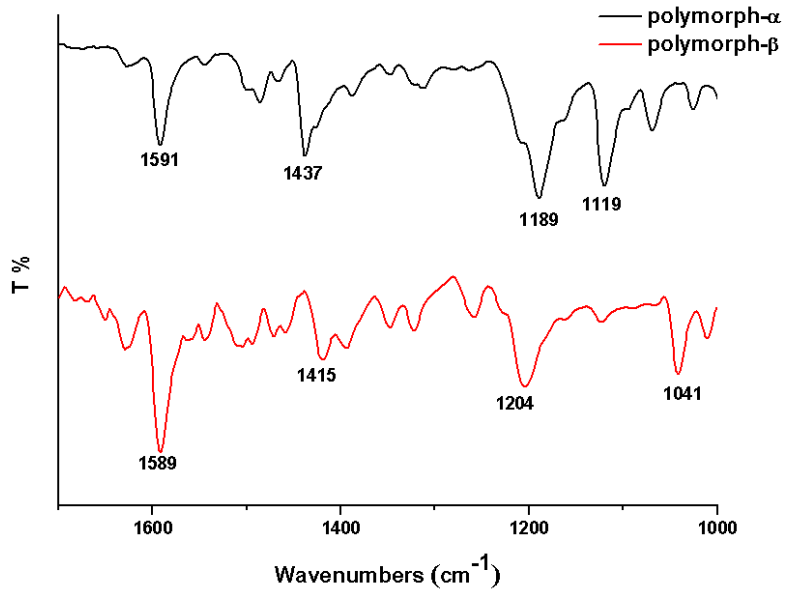


Fig. 3S Comparing IR pattern of polymorph-α and polymorph-β.

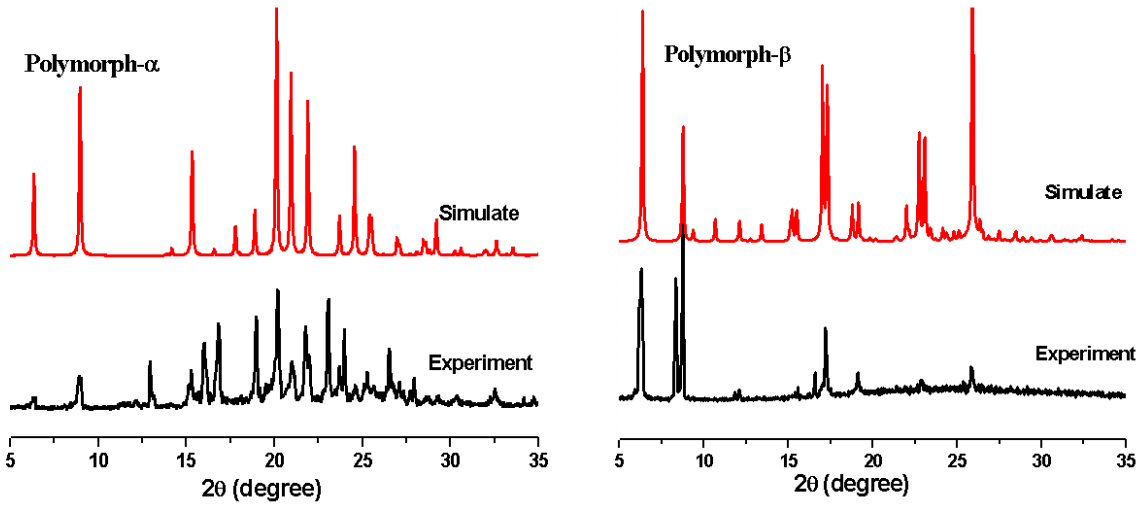


Fig. 4S As-experimental and as-simulated XRD patterns for polymorph-α and polymorph-β.

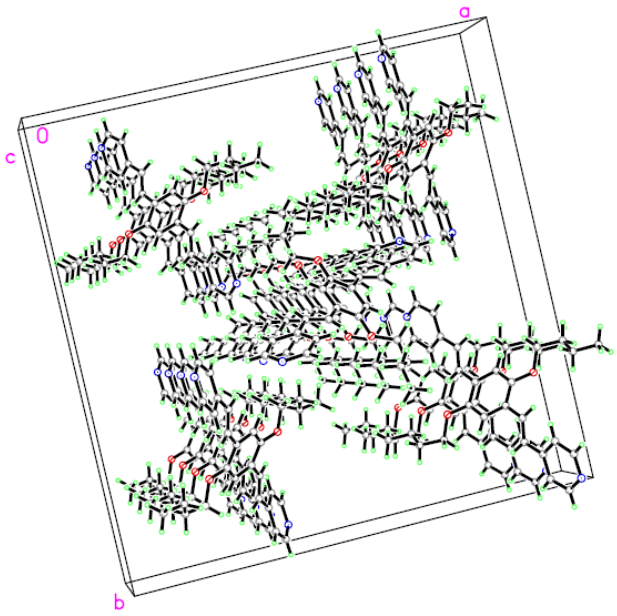


Fig. S5 Packing diagrams of polymorph-α

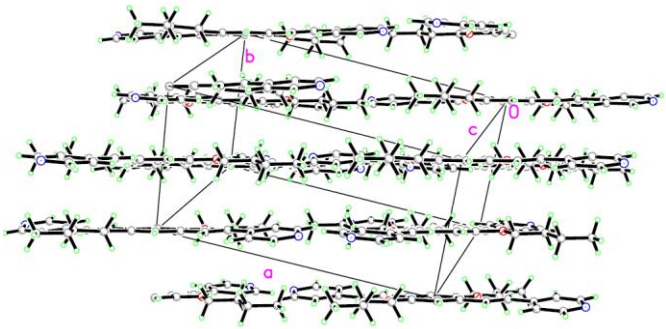
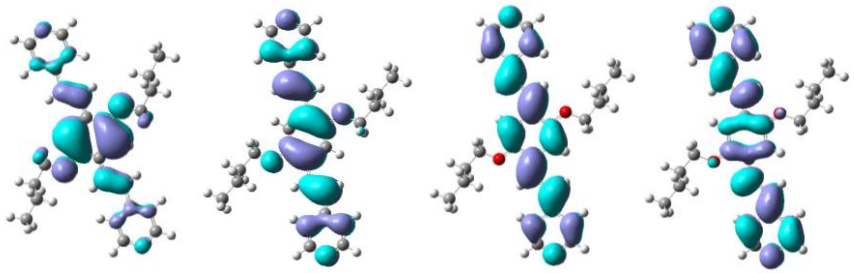


Fig. S6 Packing diagrams of polymorph-β



HOMO-1 HOMO LUMO LUMO+1

Fig. S7 Molecular orbital plots of L (The molecular structures of the species studied were calculated at TDDFT level of theory).

Table 1. Crystallographic data for polymorph-α, polymorph-β and $[Zn(phen)_3]_2\mathbf{L}(ClO_4)_4$

Compound	Polymorph-α	Polymorph-β	$[Zn(phen)_3]_2\mathbf{L}(ClO_4)_4$
Chemical Formula	$C_{28}H_{32}N_2O_2$	$C_{56}H_{64}N_4O_4$	$C_{100}H_{80}Cl_4N_{14}O_{18}Zn_2$
Formula weight	428.56	428.56	2038.32
Crystal system	Tetragonal	Triclinic	Triclinic
Space group	$I4_1/a$	$P\bar{1}$	$P\bar{1}$
a(Å)	27.908(5)	8.5234	10.976(5)
b(Å)	27.908(5)	10.7419	12.928(5)
c(Å)	6.521(5)	14.505(3)	18.049(5)
α	90.000(5)	73.507(2)	90.231(5)
β	90.000(5)	83.091(2)	92.082(5)
γ	90.000(5)	76.901(2)	113.369(5)
V(Å^3)	5079(4)	1238.0(4)	2349.0(15)
Z	8	2	2
D_{calcd}.[g·cm^{-3}]	1.121	1.150	1.441
R_1, wR_2 [$I \geq 2\sigma$ (I)]	0.0749, 0.1921	0.0841, 0.2463	0.0731, 0.2088
R_1, wR_2 *[all data]*	0.1679, 0.2462	0.1736, 0.3245	0.1143, 0.2326

Table 2. Calculated standard molar enthalpies of formation (ΔH_m) of each conformation (kJ/mol)

	Conformation 1	**Conformation 2**	**Conformation 3**	**Conformation 4**
B3LYP	-12.561037	-12.608192	-12.484656	-12.619073
BLYP	-11.912252	-11.950629	-11.826337	-11.962908
B3P86	-16.716701	-16.761831	-16.639083	-16.772874

Table 3. Solid-state photophysical properties for the crystals

Crystal	**λ_{ab} (nm)**	**λ_{ex} (nm)**	**λ_{em} (nm)**	**τ_F (ns)**
Polymorph-α	392	400	505	3.46
Polymorph-β	403	400	525	4.82
$[Zn(phen)_3]_2L(ClO_4)_4$	412	400	488	3.21